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Nonlinear softening and healing in unconsolidated granular materials: a physics-based approach

Charles Lieou

(with Eric Daub, Robert Guyer, Robert Ecke and Paul Johnson)

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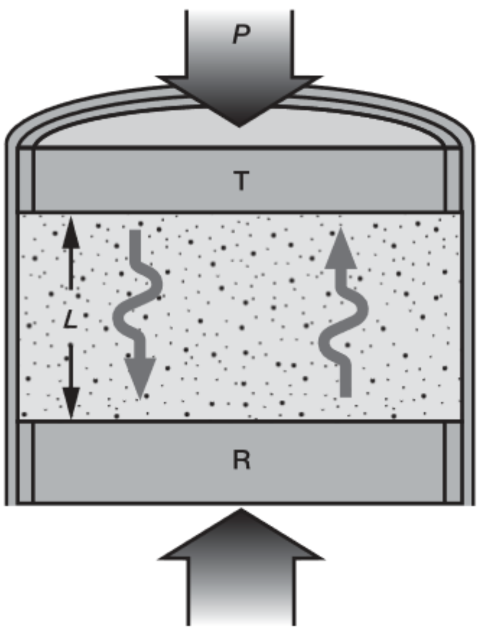
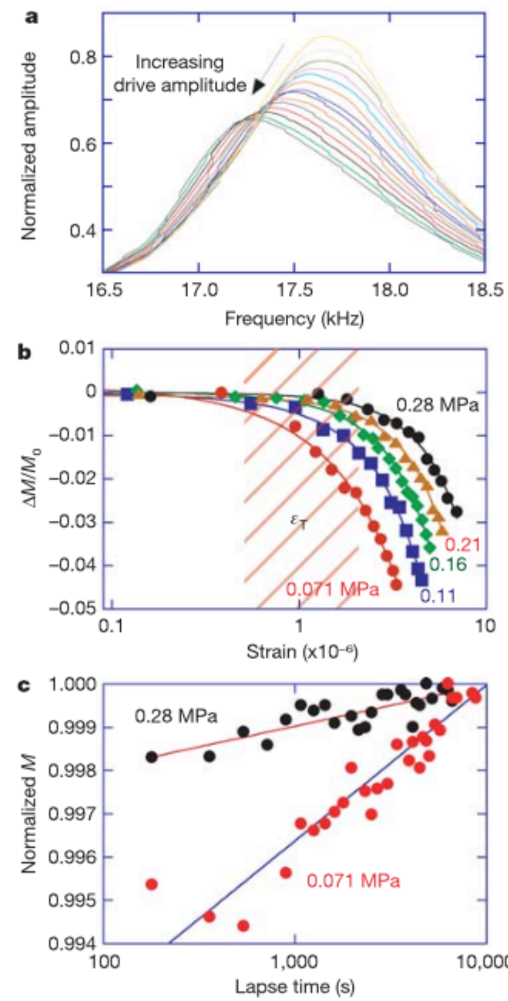
Los Alamos National Laboratory

Oct 16 2017





Outline

- Nonlinear elasticity – an overview
- STZ theory – an introduction
- ‘Linearized’ STZ theory and wave perturbation
- Probing softening and resonance shift
- Recovery of elastic modulus: need for a multi-species description

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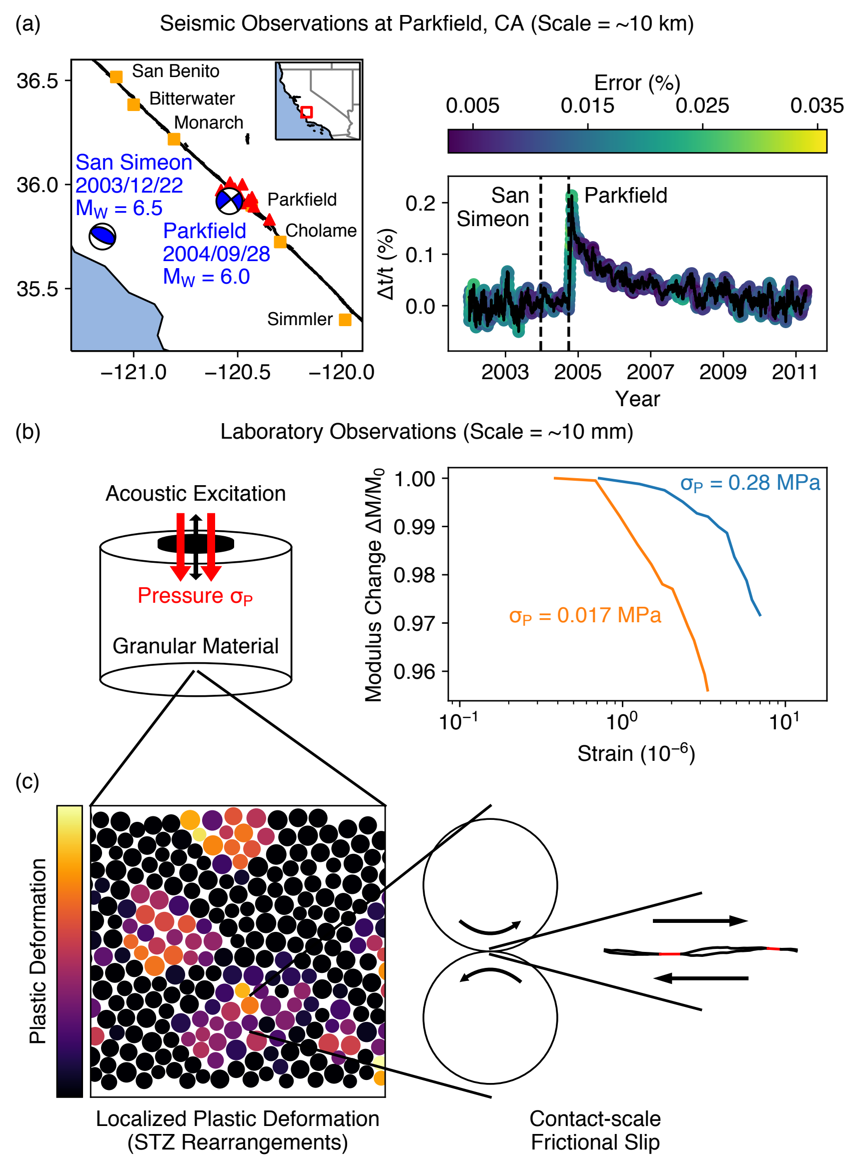
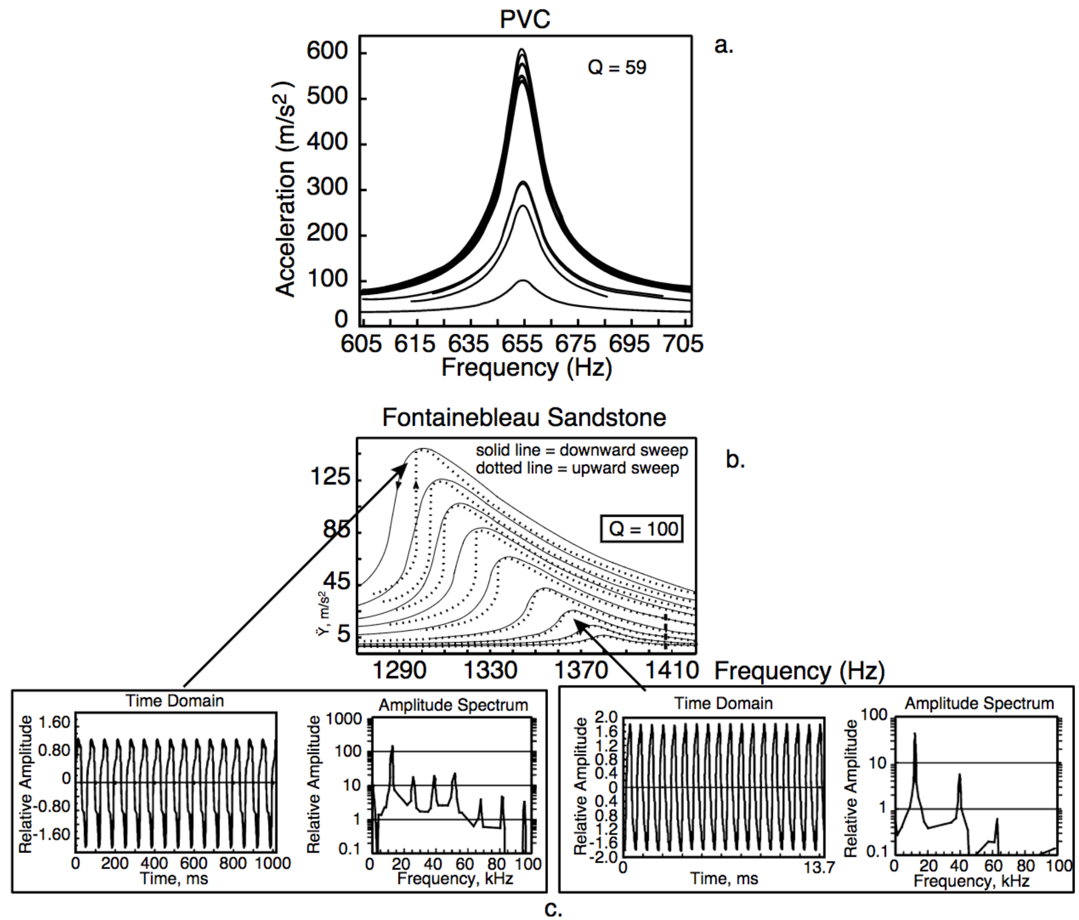
Motivation: earthquake-induced damage and post-seismic healing

- Marked drop in wave speed in the upper crust after a major earthquake is a common observation.
- The seismic wave speed takes months or even years to fully recover.
- Points to induced damage by elastic waves and slow recovery (i.e., ageing), involving complex mechanisms.
- Granular matter on faults may play important role – same observations in the laboratory.
- Unjamming transition and fluidization for unconsolidated materials in the nonlinear regime



Nonlinear elasticity

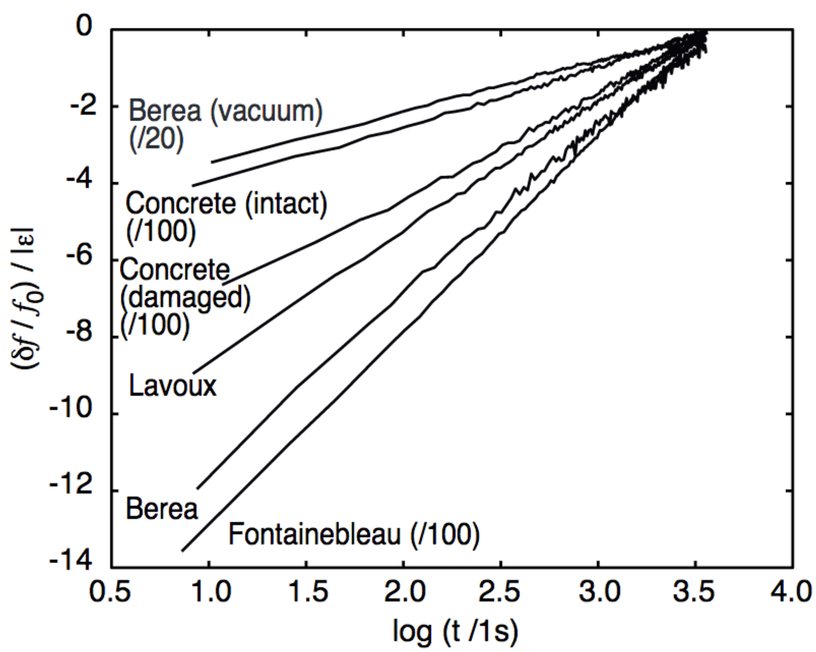
- Real materials are not ideal; defects influence mechanical behavior
- 'Fast nonlinear dynamics' is evidenced by the change of the resonance frequency, and therefore the elastic moduli, as a function of the driving amplitude.

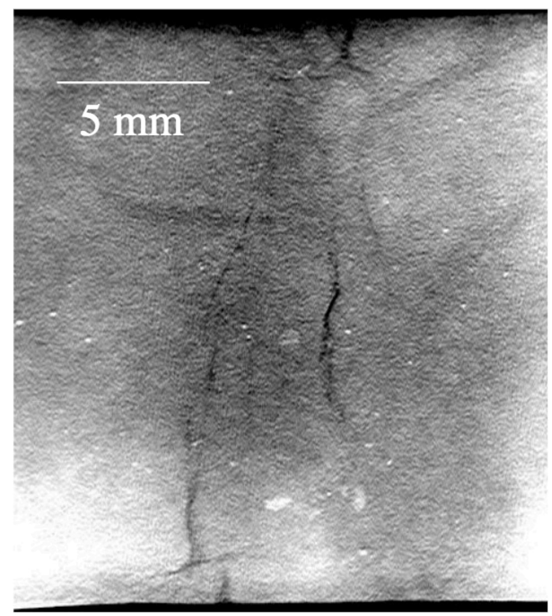


L. A. Ostrovsky and P. A. Johnson, Rivista Del Nuovo Cimento (2001)

Nonlinear elasticity

- 'Slow dynamics' seen with the gradual recovery of resonance frequency and elastic moduli upon cessation of acoustic vibration
- Nonlinear acoustics provide nondestructive probes of material damage





J. A. TenCate, E. Smith, and R. A. Guyer, PRL (2000)

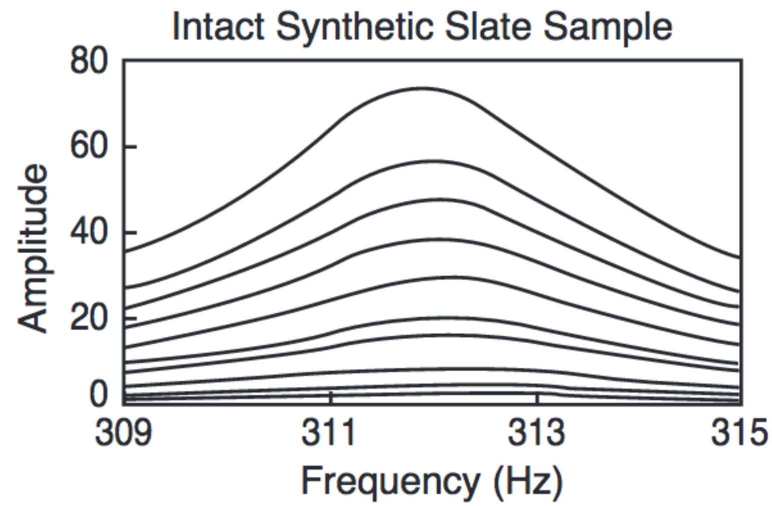
K. E-A. Van Den Abeele et al., NDT&E (2001)

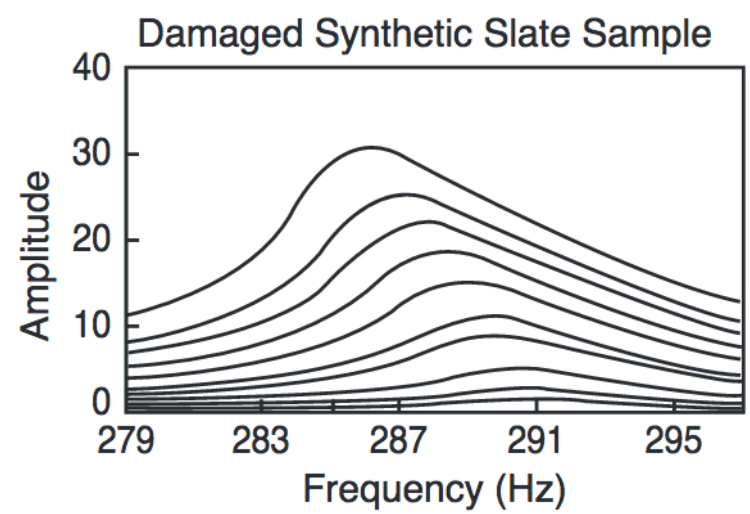
Acoustical probe of material strength and damage

- P-wave modulus M_0 is related to the speed of P-waves v through

$$v = \sqrt{\frac{M_0}{\rho_G}} = \frac{\omega_0}{k}$$

- Analogous relation between shear modulus and S-wave velocity
- Provides indirect measure of elastic moduli
- At elevated amplitudes, waves soften the material. The degree of softening reflects the amount of damage and material integrity.

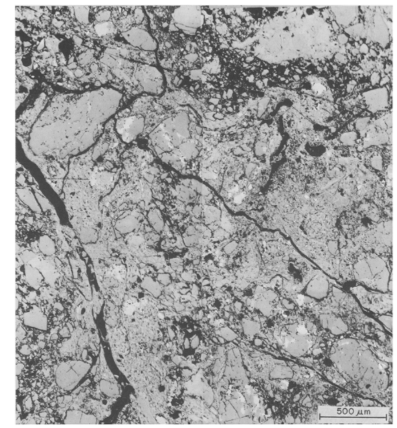




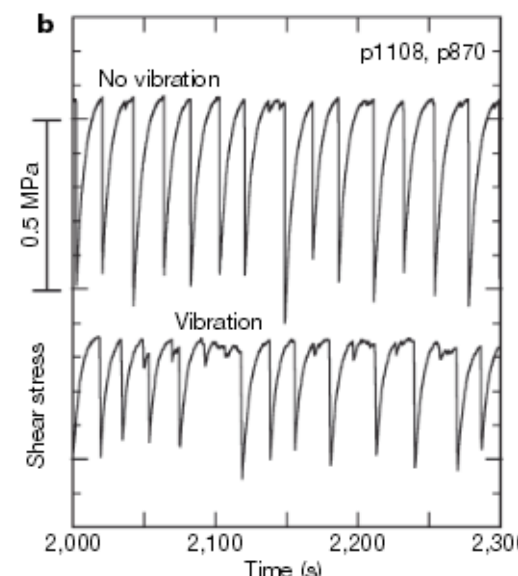
L. A. Ostrovsky and P. A. Johnson, Rivista Del Nuovo Cimento (2001)

Why study nonlinear behavior in granular media?

- Complex, strongly non-equilibrium phenomena of interest in physics and engineering
- Friction originates from response of granular layer to shear – implications for earthquake physics and control in manufacturing processes
- Acoustic emissions and seismic waves trigger earthquakes
- Other phenomena such as jamming, landslides, and avalanches



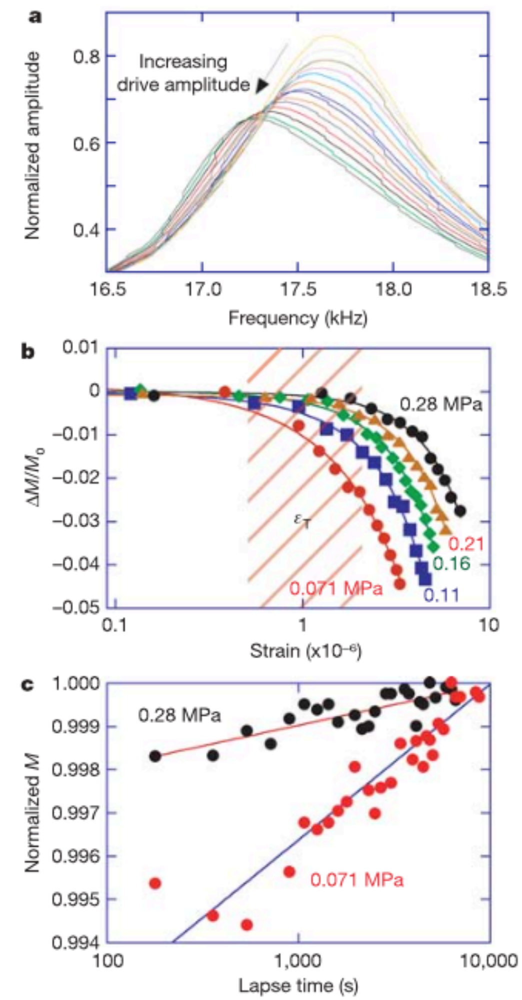
Sammis et al. (1987)



Johnson et al. (2008)

Nonlinear behavior in glass bead packs

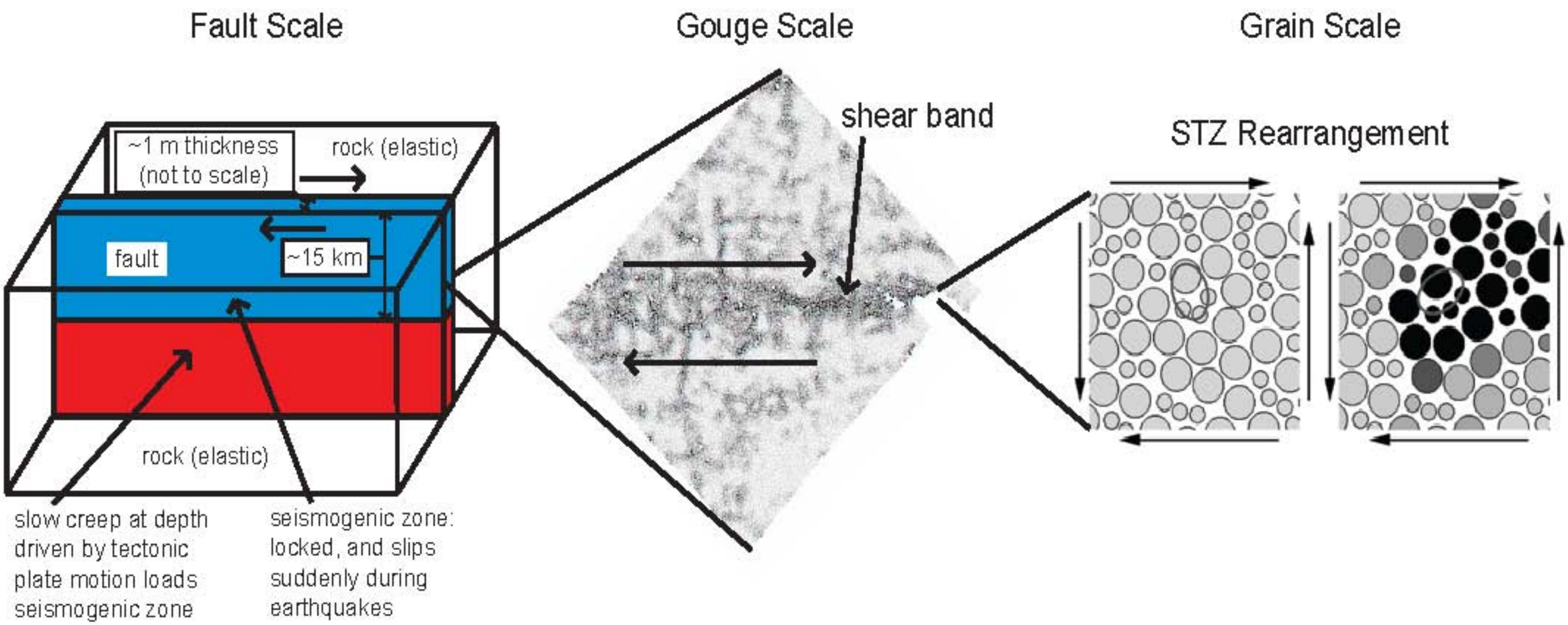
- Glass bead packs display nonlinear acoustic behavior, as in other consolidated and unconsolidated materials, yet are easier to handle in the laboratory
- We attribute deformation and plasticity to rearranging clusters of grains called shear transformation zones (STZs)
- Goal: to properly understand softening and resonance shift in a granular material subject to wave perturbation.



P. A. Johnson and X. Jia, Nature (2005)

Multiscale modeling

- To connect small-scale physics to large-scale phenomena



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- Nonlinear elasticity – an overview
- STZ theory – an introduction
- ‘Linearized’ STZ theory and wave perturbation
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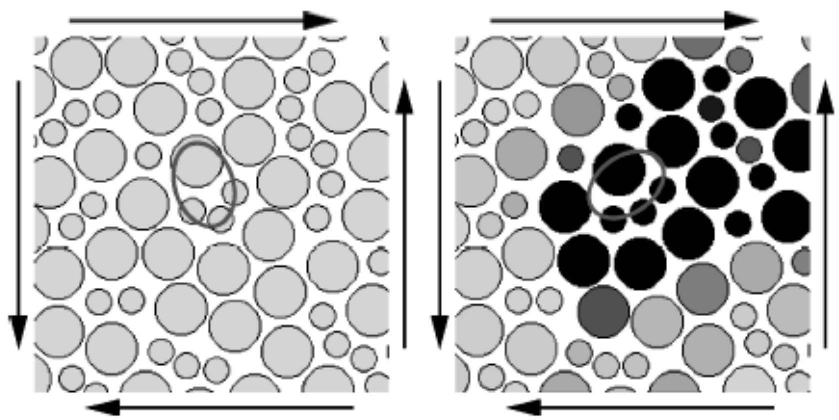
- Recovery of elastic modulus: need for a multi-species description

[C. K. C. Lieou and J. S. Langer, PRE 85, 061308 (2012)]

STZ's – microscopic description of shear deformation in granular media

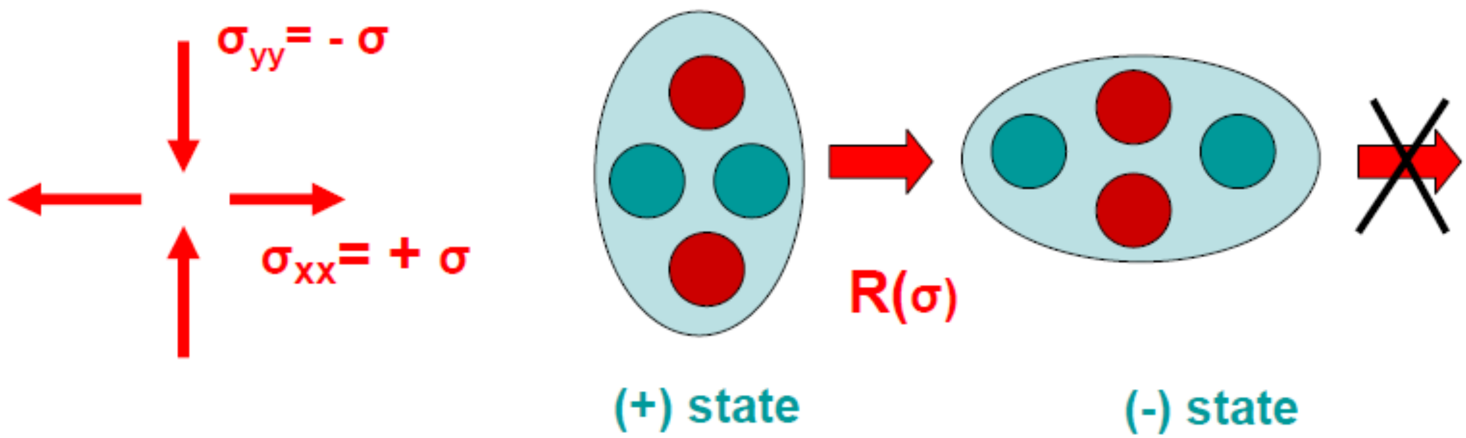
- Starting point: molecular/granular rearrangements lead to deformation of solids
- Shear transformation zones are local flow defects susceptible to shear deformation and contact change



[M. L. Falk and J. S. Langer, PRE 57, 7192 (1998)]

STZ theory: a short introduction

- To a good approximation, STZs come in two states; stable, and unstable, with respect to the deviatoric stress.



$$\boxed{\tau}\dot{N}_\pm = \boxed{\mathcal{R}(\pm\sigma)N_\mp - \mathcal{R}(\mp\sigma)N_\pm} + \boxed{\Gamma\left(Ne^{-1/\chi} - N_\pm\right)}$$

Inertial time scale (or inverse attempt frequency)

stress-driven transitions between the two possible states

noise-driven creation and annihilation of STZ defects

STZ theory: a short introduction

- The STZ density at the stationary state

$$\Lambda \equiv \frac{N_+ + N_-}{N} = 2e^{-1/\chi}$$

  is given by a thermodynamically-defined 'compactivity' χ with structural origins, reflecting disorder in the granular packing

- Plastic deformation when STZs 'flip' from one state to another, i.e., nonaffine rearrangement of grains (in the sense of change in contacts)

$$\dot{\epsilon}^{\mathrm{pl}} = \frac{\epsilon_0}{\tau N} e^{-1/\chi} \left(\mathcal{R}(\sigma) N_- - \mathcal{R}(-\sigma) N_+ \right)$$

STZ theory: a short introduction

- STZ orientational bias

$$m \equiv \frac{N_+ - N_-}{N_+ + N_-}$$

- Define combinations of rate factors

$$\mathcal{C}(\sigma) = \frac{\mathcal{R}(\sigma) + \mathcal{R}(-\sigma)}{2}; \quad \mathcal{T}(\sigma) = \frac{\mathcal{R}(\sigma) - \mathcal{R}(-\sigma)}{\mathcal{R}(\sigma) + \mathcal{R}(-\sigma)}$$

- After change of variables

$$\begin{aligned} \tau \dot{m} &= 2\mathcal{C}(\sigma)\left(\mathcal{T}(\sigma) - m\right)\left(1 - \frac{m\sigma}{\sigma_0}\right); \\ \tau \dot{\epsilon}^{\mathrm{pl}} &= 2\epsilon_0 e^{-1/\chi}\mathcal{C}(\sigma)\left(\mathcal{T}(\sigma) - m\right). \end{aligned}$$

- It can be shown that $\mathcal{T}(\sigma) = \tanh[\epsilon_0 \sigma / (\epsilon_Z \sigma_p \chi)]$ (σ_p = pressure)

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[C. K. C. Lieou, E. G. Daub, R. A. Guyer, and P. A. Johnson, J. Geophys. Res. Solid Earth, in press]

Wave perturbation: linearize STZ equations

- Under wave perturbation with amplitude small enough compared to the external load, σ refers to the oscillatory component of the stress associated with the wave (e.g., pressure wave)
- Linearize STZ equations around the small quantities m and σ:

$$\begin{aligned} \tau \dot{m} &= 2R_0 \left(\frac{\Omega \sigma}{\chi} - m \right); \\ \tau \dot{\epsilon}^{\mathrm{pl}} &= 2R_0 \epsilon_0 e^{-1/\chi} \left(\frac{\Omega \sigma}{\chi} - m \right) \end{aligned}$$

Here $\Omega \equiv \epsilon_0 / (\epsilon_Z \sigma_p)$

Wave perturbation: linearize STZ equations

- Combine these with the equations of motion:

$$\dot{\sigma} = \boxed{M_0}(\dot{\epsilon} - \dot{\epsilon}^{\rm pl}),$$

Unperturbed modulus at max. packing fraction

$$\rho_G \ddot{u} = \frac{\partial \sigma}{\partial x} + \boxed{F,} \qquad \boxed{\epsilon = \frac{\partial u}{\partial x}}$$

External forcing

Total strain in terms of displacement

- Use the ansatz

$$\begin{aligned} u &= \hat{u} e^{i(kx-\omega t)}; \\ \sigma &= \hat{\sigma} e^{i(kx-\omega t)}; \\ m &= \hat{m} e^{i(kx-\omega t)}; \\ F &= \hat{F} e^{i(kx-\omega t)}. \end{aligned}$$

Wave perturbation: linearize STZ equations

- The result is

$$
\begin{aligned}
-\omega^2 \rho_G \hat{u} &= ik\hat{\sigma} + \hat{F}; \\
-i\omega\hat{m} &= \alpha\left(\frac{\Omega\hat{\sigma}}{\chi} - \hat{m}\right); \\
-i\omega\hat{\sigma} &= M_0\left[k\omega\hat{u} - \alpha\epsilon_0 e^{-1/\chi}\left(\frac{\Omega\hat{\sigma}}{\chi} - \hat{m}\right)\right]
\end{aligned}
$$

where $\alpha \equiv 2R_0/\tau$.

- Eliminating m and σ gives

$$
\hat{F} = \rho_G \frac{(\omega_0^2\alpha - \omega^2\beta) - i\omega(\omega_0^2 - \omega^2)}{\beta - i\omega}\hat{u}
$$

with $\beta \equiv \alpha(1 + M_0\epsilon_0\Omega e^{-1/\chi}/\chi)$, and $v = \sqrt{\frac{M_0}{\rho_G}} = \frac{\omega_0}{k}$.

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Response function

- The relation between drive amplitude F (corresponding to, e.g, voltage) and response amplitude u

$$\hat{F} = \rho_G \frac{(\omega_0^2 \alpha - \omega^2 \beta) - i\omega(\omega_0^2 - \omega^2)}{\beta - i\omega} \hat{u}$$

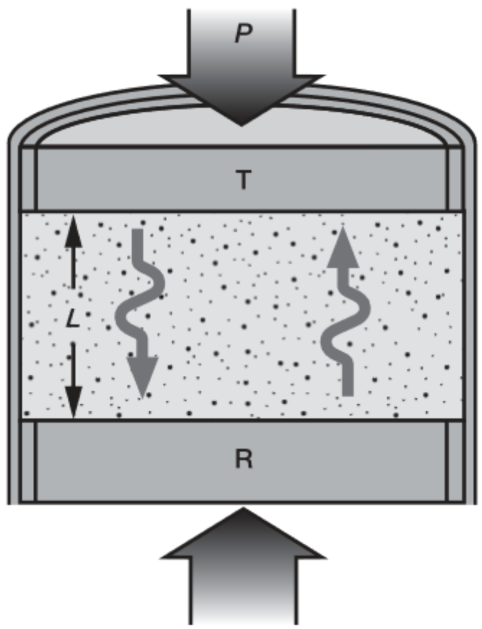
prompts us to define the 'response function'

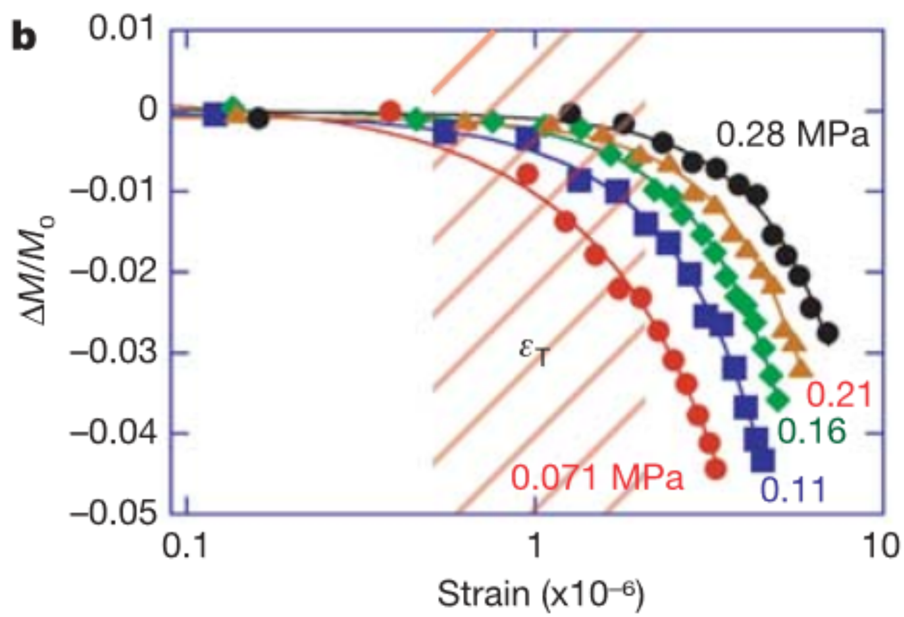
$$A(\omega) \equiv \frac{\beta - i\omega}{(\omega_0^2 \alpha - \omega^2 \beta) - i\omega(\omega_0^2 - \omega^2)}$$

- The norm of $A(\omega)$ gives the normalized strain amplitude; probing $A(\omega)$ gives the tuning curves and resonance peaks.

Modulus softening

- Experiments show modulus softening due to external acoustic vibrations
- External vibrations at single frequency roughly equivalent to oscillatory driving





[Johnson and Jia, Nature, 2005]

Modulus softening

- The ‘softened’ modulus M is given in terms of the resonance frequency ω_{res} and the system size H by

$$\omega_{\text{res}}^2 = \left(\frac{\pi}{H}\right)^2 \frac{M}{\rho_G}$$

- What controls the resonance frequency? Recall that

$$A(\omega) \equiv \frac{\beta - i\omega}{(\omega_0^2\alpha - \omega^2\beta) - i\omega(\omega_0^2 - \omega^2)}$$

$$\beta \equiv \alpha(1 + M_0\epsilon_0\Omega e^{-1/\chi}/\chi)$$

If the compactivity χ varies with the strain amplitude (reasonable), the resonance frequency may shift!

Modulus softening

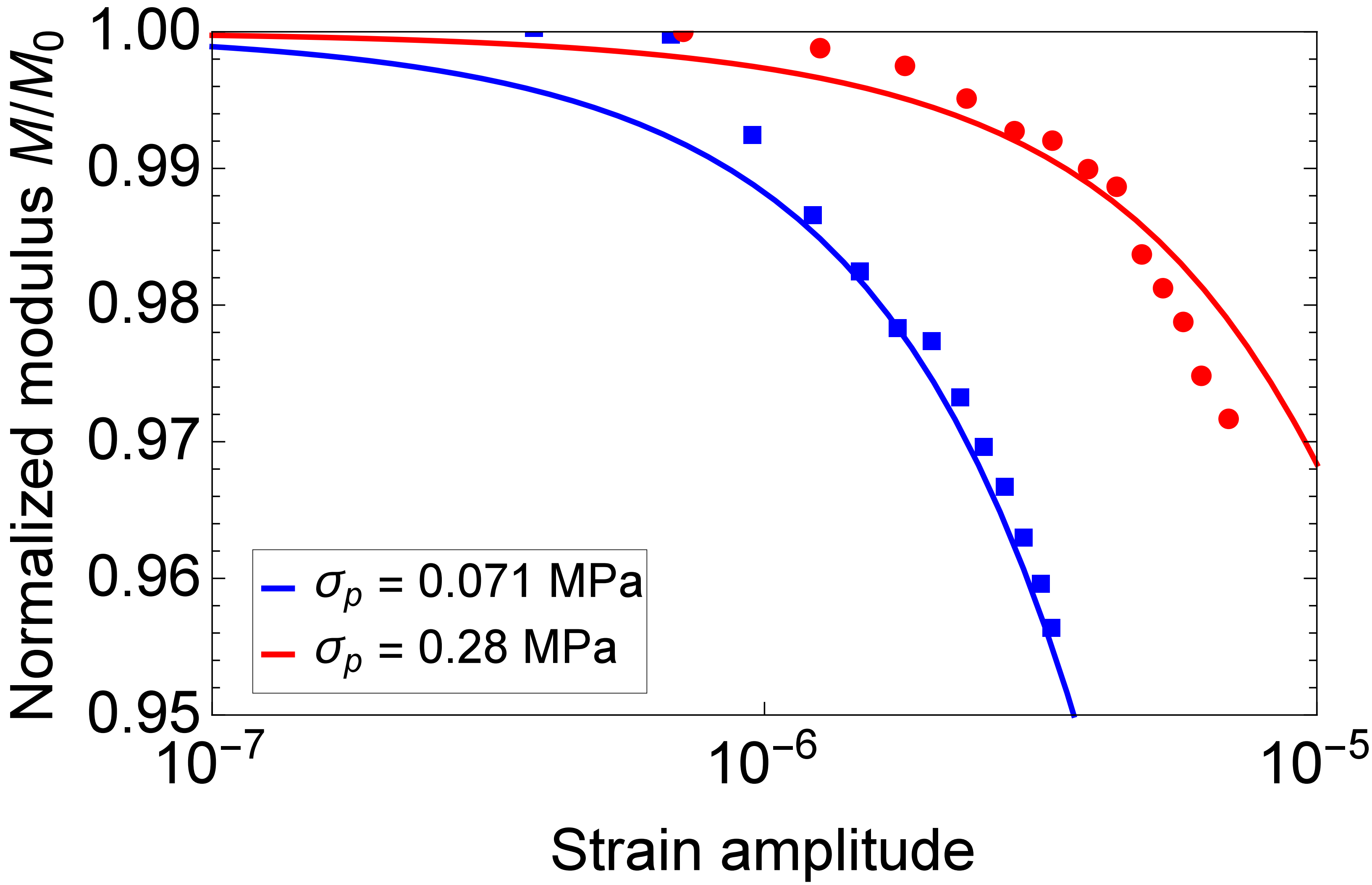
- Intuition: the compactivity χ must be an increasing function of the strain amplitude.
- More strain => Higher compactivity => More STZ defects => Granular material becomes softer!
- To fit with the experimental softening data, use the ansatz

$$\chi(\epsilon_{\mathrm{dyn}}) = \chi_0 + \chi_1 \tanh\left[\left(\frac{\sigma_t}{\boxed{\sigma_p}}\right)^{2/3} \boxed{\epsilon_{\mathrm{dyn}}}\right]$$

Applied load

Dynamic strain amplitude

Modulus softening



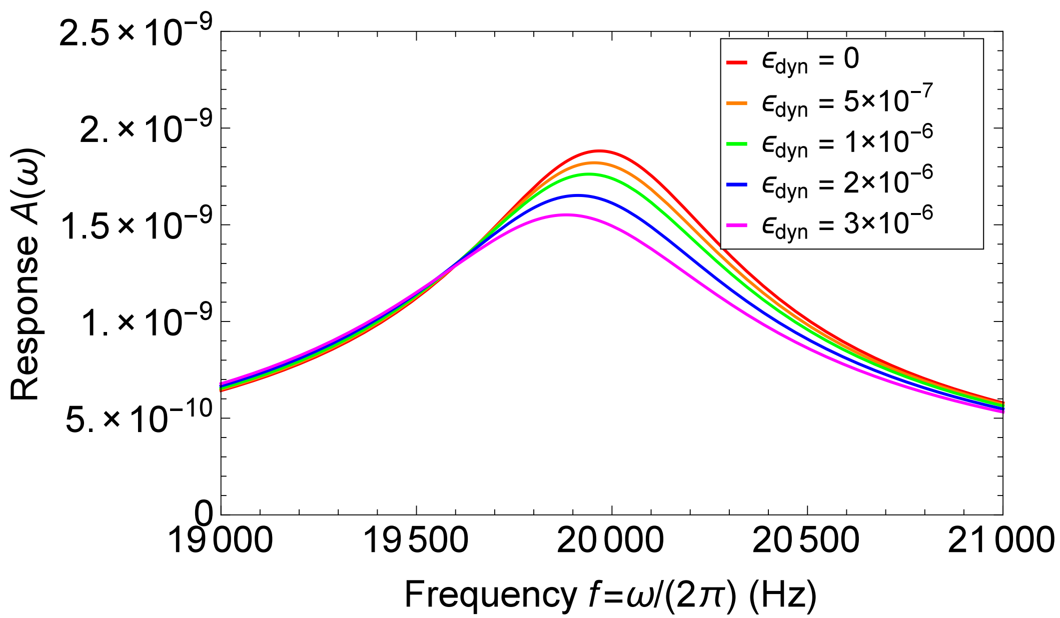
(Data points: experiment; curves: theoretical results)

Resonance shift

- By directly computing the response function

$$A(\omega) \equiv \frac{\beta - i\omega}{(\omega_0^2\alpha - \omega^2\beta) - i\omega(\omega_0^2 - \omega^2)}$$

we can get the tuning curves:



Attenuation

- We can compute the attenuation Q-factor in the nonlinear regime from the linear Q, computed from the full-width-at-half-maximum of the square norm (power) of the response function:

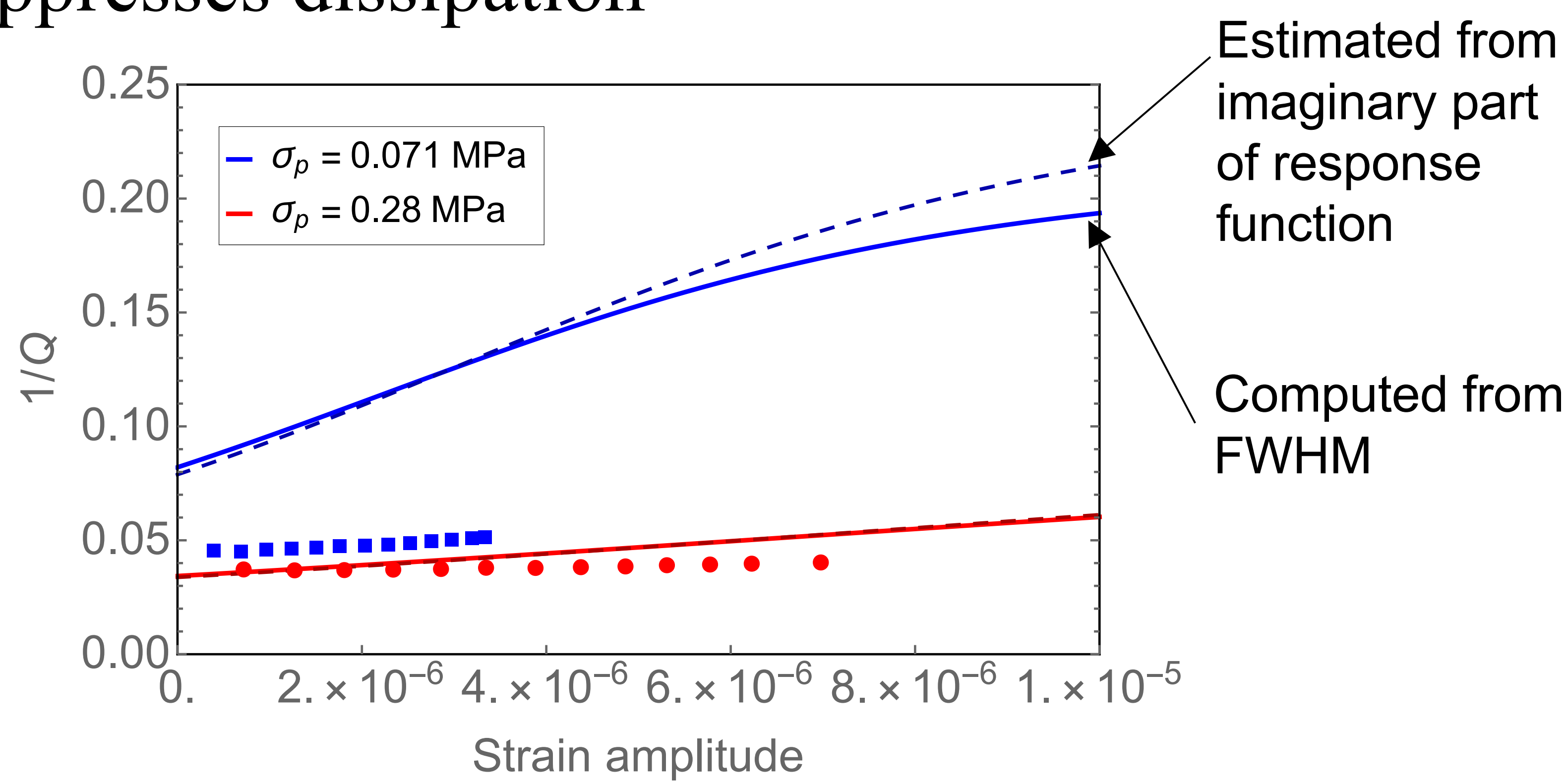
$$Q_0 = \frac{\omega_{\mathrm{res}}(\epsilon_{\mathrm{dyn}} = 0)}{\Delta\omega} \qquad\qquad Q = Q_0 \frac{|A(\omega_{\mathrm{res}})|}{|A(\omega_{\mathrm{res}}(\epsilon_{\mathrm{dyn}} = 0))|}$$

- Or estimate it from the response function directly:

$$Q_{\mathrm{est}} = \frac{(\beta^2 + \omega_{\mathrm{res}}^2))\omega_{\mathrm{res}}^2}{(\beta - \alpha)\omega_{\mathrm{res}}\omega_0^2}$$

Attenuation

- 1/Q increases almost linearly with increasing strain amplitude
- Larger for smaller load level – sensible as higher load suppresses dissipation



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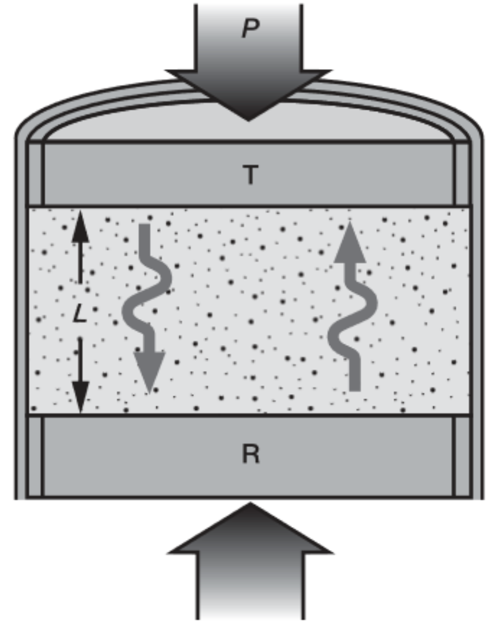
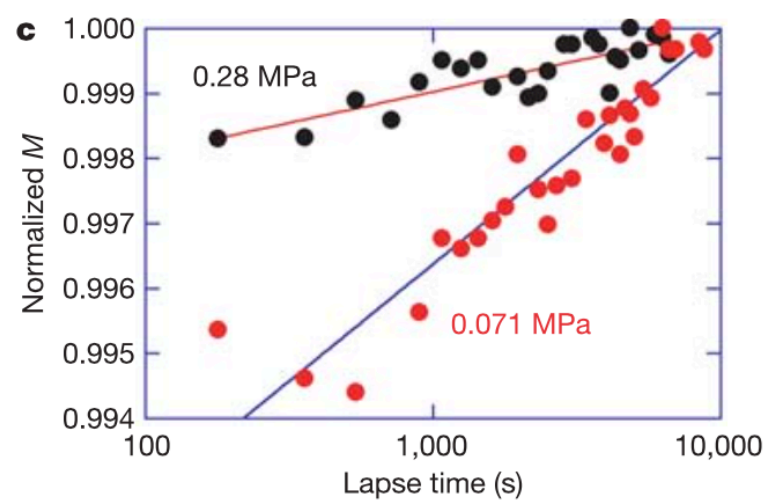
  [C. K. C. Lieou, E. G. Daub, R. E. Ecke, and P. A. Johnson, J. Geophys. Res. Solid Earth, in press]

Modulus recovery

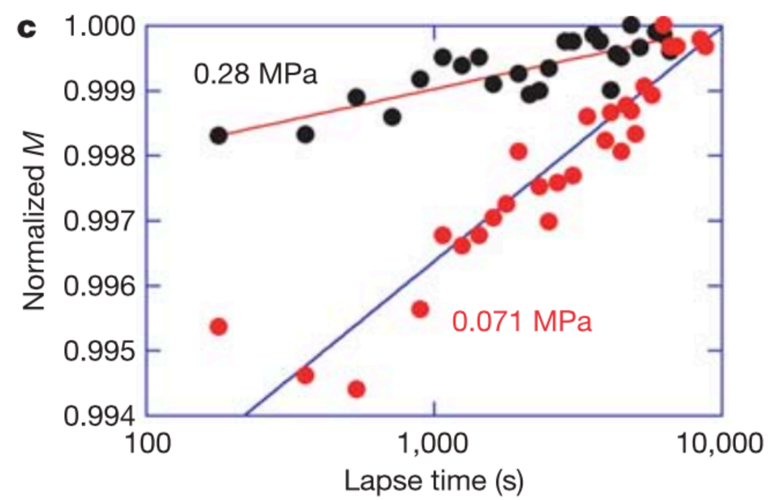
- Experiments indicate that the P-wave modulus slowly recovers as a function of time after the cessation of external acoustic strain, with log-linear dependence.
- We propose to infer modulus recovery from strain recovery.





Need for a multi-species description

- At large stresses and strain rates, a single-species STZ formulation suffices; STZs with low activation barriers are annihilated before they can transition from one state to another and contribute to irreversible deformation.
- In aging experiments, STZs with a broad spectrum of time scales play a role; slow STZs become prominent.



Multi-species STZ theory

- From now on, focus on compressional stress configuration
- Insert dependence on barrier height Δ into the STZ dynamical equations:

$$\tau \dot{N}_\pm(\Delta) = \mathcal{R}(\pm\sigma_C, \Delta) N_\mp(\Delta) - \mathcal{R}(\mp\sigma_C, \Delta) N_\pm(\Delta)$$
$$+ \rho \left[\frac{N^{\text{eq}}(\Delta)}{2} - N_\pm(\Delta) \right]$$

Vibration intensity (retained for bookkeeping)

Multi-species STZ theory

- Transition rate increases with dimensionless compactivity $\chi = X / v_Z$:

$$\mathcal{R}(\sigma_C, \Delta) = R_0(\sigma_C, \Delta) \exp\left[-\frac{\Delta}{\epsilon_Z \chi} \exp\left(-\frac{\epsilon_0 \sigma_C}{\sigma \Delta}\right)\right]$$

- Define the STZ density and orientational bias

$$\Lambda(\Delta) = \frac{N_+(\Delta) + N_-(\Delta)}{N}; \quad m(\Delta) = \frac{N_+(\Delta) - N_-(\Delta)}{N_+(\Delta) + N_-(\Delta)},$$

and the symmetric and antisymmetric transition rates

$$\mathcal{C}(\sigma_C, \Delta) = \frac{\mathcal{R}(\sigma_C, \Delta) + \mathcal{R}(-\sigma_C, \Delta)}{2}; \quad \mathcal{T}(\sigma_C, \Delta) = \frac{\mathcal{R}(\sigma_C, \Delta) - \mathcal{R}(-\sigma_C, \Delta)}{\mathcal{R}(\sigma_C, \Delta) + \mathcal{R}(-\sigma_C, \Delta)}$$

Multi-species STZ theory

- Then the plastic strain rate becomes

$$\dot{\epsilon}^{\rm pl} = \frac{2\epsilon_0}{\tau} e^{-1/\chi} \int d\Delta p(\Delta) \mathcal{C}(\sigma_C, \Delta) \left[\mathcal{T}(\sigma_C, \Delta) - m(\Delta)\right].$$

- Linearizing around the small stress, we have

$$\dot{\epsilon}^{\rm pl} = \frac{\epsilon_0}{\tau} e^{-1/\chi} \int d\nu \tilde{p}(\nu) \nu \left[\frac{\epsilon_0 \sigma_C}{\epsilon_Z \sigma \chi} - \tilde{m}(\nu)\right]$$

where we have changed representation from the barrier height Δ to the transition rate variable ν:

$$\nu(\Delta) \equiv 2\mathcal{C}(0, \Delta) = 2R_0(0, \Delta) e^{-\Delta/\chi}$$

- Also, $$\tau \dot{\tilde{m}} = \frac{\epsilon_0 \nu}{\epsilon_Z \sigma \chi} \sigma_C - (\nu + \rho) \tilde{m}(\nu).$$

Barrier-height distribution

- We need to know the barrier-height distribution in order to carry out further calculations and interpret experimental findings.
- Δ is measured *downward* from some reference volume.
- Ignoring regularity for now, $p(\Delta)$ should look like

$$p(\Delta) \propto e^{\Delta/\bar{\Delta}}$$

or

$$\tilde{p}(\nu) \propto \nu^{-(1+\zeta)}$$

Barrier-height distribution

- The large-Δ, small-ν distribution must be cut off at some threshold Δ^* or ν^*.
- In that limit, we propose

$$p(\Delta) \propto e^{-\Delta/\tilde{\Delta}_1}, \qquad \tilde{p}(\nu) \propto \nu^{-(1-\zeta_1)}$$

- Combining the results in the two limiting regimes,

$$\tilde{p}(\nu) = \frac{A}{\nu[(\nu/\nu^*)^{\zeta} + (\nu^*/\nu)^{\zeta_1}]}.$$

- The exponents may be determined from the experimental measurements.

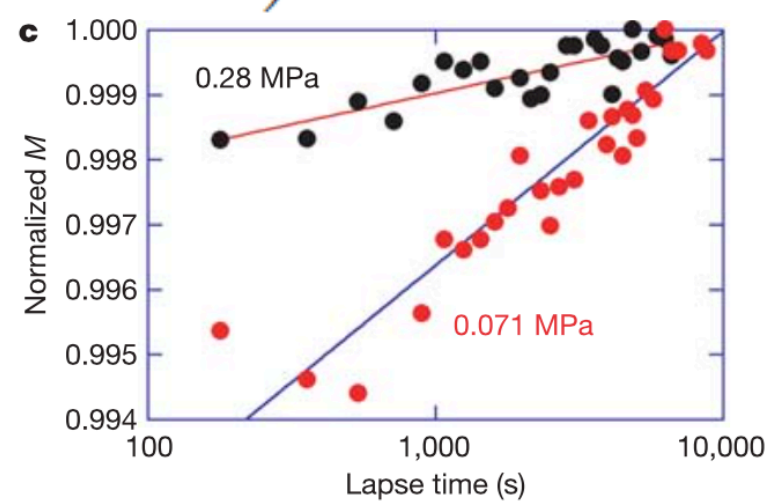
Modulus recovery

- Modulus recovery from strain recovery at fixed stress σ:

$$M(t) = \frac{\sigma}{\epsilon(t) - \epsilon^{\mathrm{pl}}(t)} = \frac{\sigma M_0}{\sigma - M_0 \epsilon^{\mathrm{pl}}(t)}$$

- At zero vibration intensity:

$$\dot{\epsilon}^{\mathrm{pl}} = \frac{\epsilon_0}{\tau} e^{-1/\chi} \int d\nu \tilde{p}(\nu) \nu \left(\frac{\epsilon_0}{\epsilon_Z \chi} \operatorname{sgn}(\sigma) - \tilde{m}_0 \right) e^{-\nu t/\tau}$$



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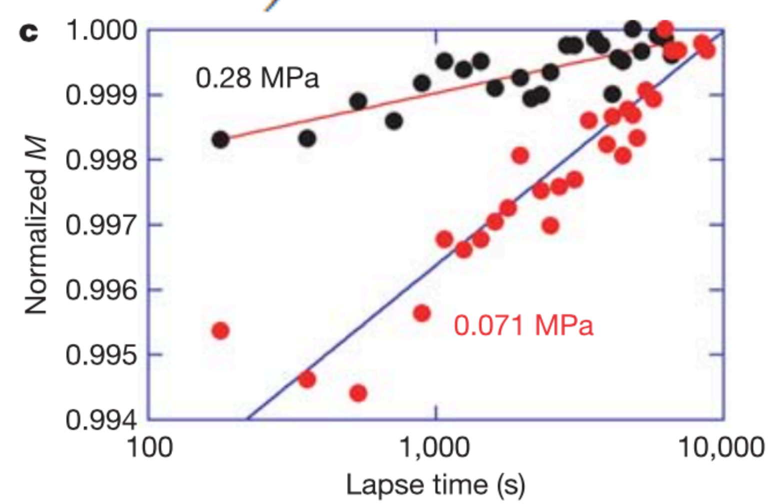
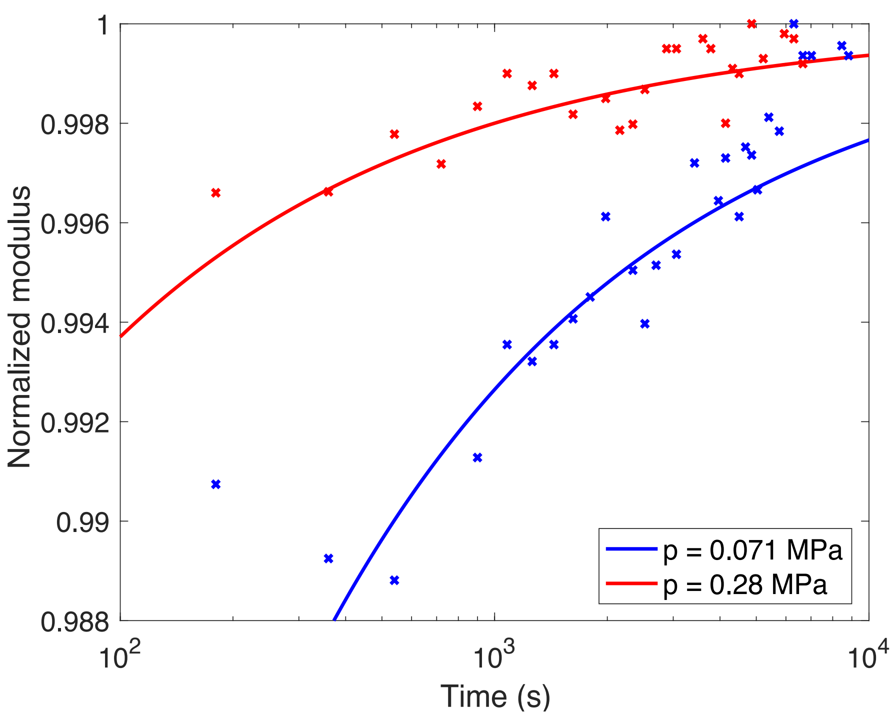
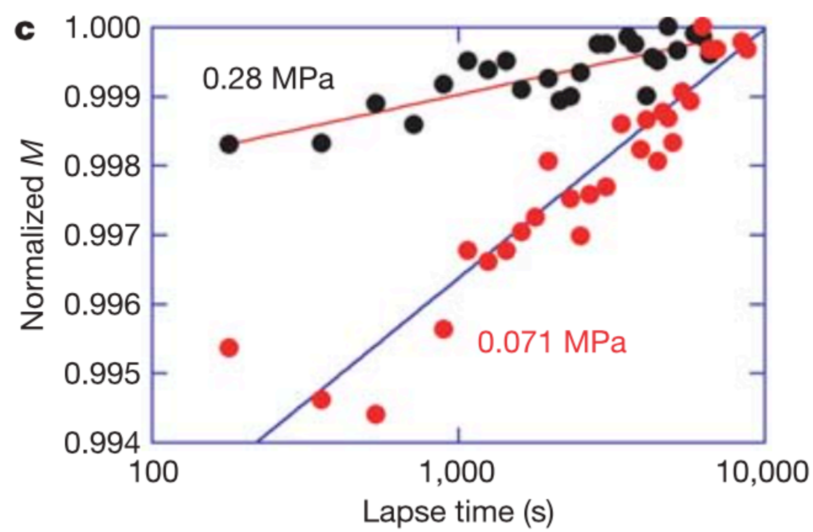


Modulus recovery

$$\tilde{p}(\nu) = \frac{A}{\nu[(\nu/\nu^*)^{\zeta} + (\nu^*/\nu)^{\zeta_1}]}.$$

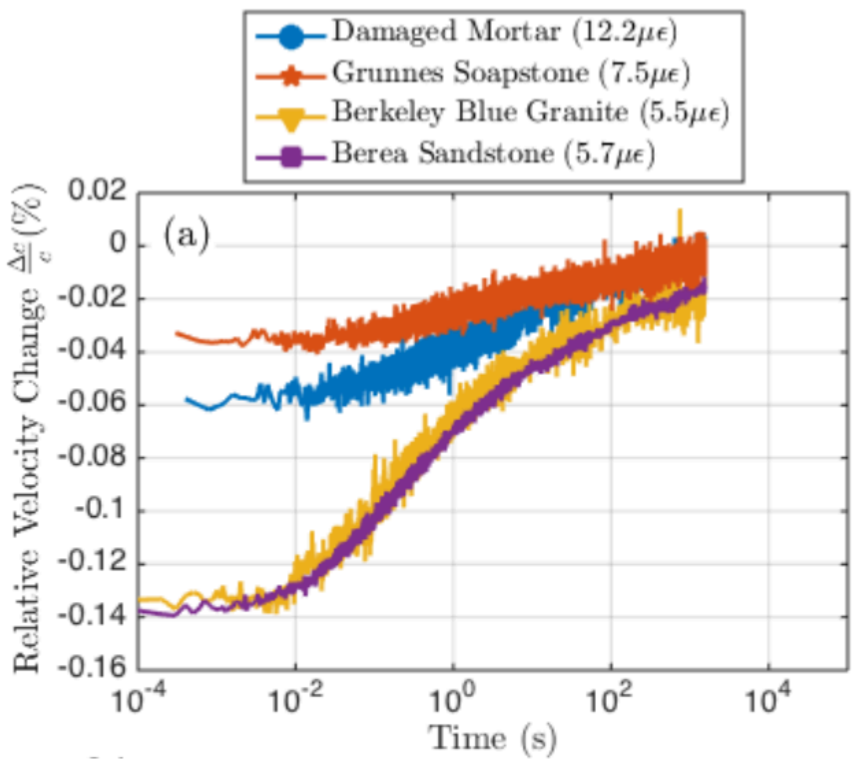
- At long times, slow STZs (small ν) dominate.
- Need to choose $\zeta_1 = ½$ to fit logarithmic recovery.





Short-time behavior

- Sandstone dynamic acousto-elasticity experiments indicate characteristic recovery time ~ 0.1 s during which modulus stays around perturbed value. [Shokouhi et al., 2017, submitted]
- Guess: same type of behavior in unconsolidated glass beads (no data yet)



Short-time behavior

$$\tilde{p}(\nu) = \frac{A}{\nu[(\nu/\nu^*)^{\zeta} + (\nu^*/\nu)^{\zeta_1}]}.$$

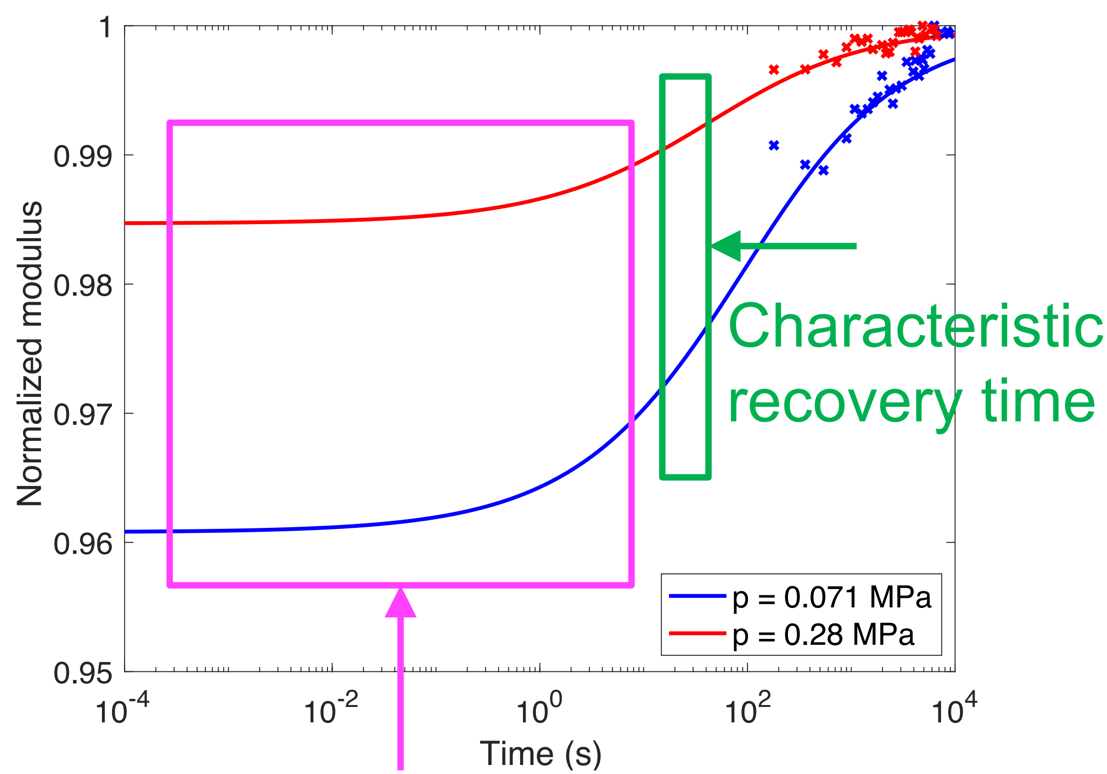
- Guess: same type of behavior in unconsolidated glass beads (no data yet)
- Choose $\zeta = \zeta_1 = ½$ for which there is an analytic solution

$$\frac{M(t)}{M_0} = \left[1 + \frac{M_0}{\sigma}\,\mathrm{sgn}(\sigma)\frac{\epsilon_0^2}{\epsilon_Z}\frac{e^{-1/\chi}}{\chi}e^{\nu^* t/\tau}\,\mathrm{erfc}\left(\sqrt{\frac{\nu^* t}{\tau}}\right)\right]^{-1}.$$

Short-time behavior

$$\frac{M(t)}{M_0} = \left[1 + \frac{M_0}{\sigma}\,\mathrm{sgn}(\sigma)\frac{\epsilon_0^2}{\epsilon_Z}\frac{e^{-1/\chi}}{\chi}e^{\nu^* t/\tau}\,\mathrm{erfc}\left(\sqrt{\frac{\nu^* t}{\tau}}\right)\right]^{-1}.$$

- A variety of combinations of χ and ν^* reproduce the correct long-time behavior.
- Characteristic recovery time of τ/ν^* helps constrain these parameters.



Short-time regime predictions to be validated by future experiment?

Concluding remarks

- STZ theory describes defect dynamics and plasticity in granular materials
- Addresses inadequacies in other empirical theories
- Compactivity – describing structural disorder – is key variable that controls defect density
- Coupling linearized STZ theory with wave equations generates modulus softening and downwards resonance shift with increasing strain amplitude
- Shows definitely that STZ defects are responsible for softening and dissipative, nonlinear behavior

Concluding remarks

- To describe long-time relaxation and healing, we need a model that accounts for a spectrum of time scales of the plasticity carriers (STZs in this case)
- Generic assumption on barrier distribution and STZ spectrum reproduces experimentally-observed modulus recovery
- Characteristic recovery time reveals information about the STZ spectrum

Future outlook

- Extension to consolidated, amorphous rock materials?
- Motion of single grains – calculation of diffusion constant?
- Dynamic acousto-elasticity experiments to probe short-time regime – theory validation?
- Generalization to pronounced, shear wave induced softening (X. Jia et al.)?
- Polycrystalline rock materials – role of point and line defects (dislocations)?

Appendix:
Backup slides

Big picture: Statistical thermodynamics

- According to the first law of thermodynamics, the (dimensionless) compactivity obeys an equation of the form

$$\boxed{\epsilon_1}\dot{\chi} = \boxed{\mu\dot{\gamma}^{\rm pl}} - \boxed{\mathcal{K}(\chi,\theta)(\chi-\theta)}$$

effective volume expansion coefficient

rate of plastic work of deformation (normalized by pressure)

coupling to kinetic-vibrational degrees of freedom by noise sources, that relax the configurational subsystem to state θ

- Presence of other noise sources (tapping ρ, and friction ξ) changes the steady-state behavior.

Microscopic model

- Statistical thermodynamics is sufficient to account for qualitative behavior.
- The rest is microscopic detail that quantitatively connects the volume V, the compactivity χ, and the shear rate q.
- Microscopic model consists of STZ's and misalignments